REPORT DOCUMENTATION PAGE	AFRL-SR-AR-TR-04-0205

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
18-03-2004	Final	Dec 2000-Nov 2003

4. TITLE AND SUBTITLE	
"Fully Automatic hp-Adaptive Simulations for Maxwell's Equations"	5a. CONTRACT NUMBER: F49620-01-1-0043
	5b. GRANT NUMBER: AFOSR/PK3
	5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S): Leszek Demkowicz	5d. PROJECT NUMBER
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)	8. PERFORMING ORGANIZATION REPORT NUMBER
Institute for Computational Engineering and Sciences, the University of Texas at Austin	

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
Air Force Office of Scientific Research	AFOSR
	11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT

Unrestricted

13. SUPPLEMENTARY NOTES

Final Report

14. ABSTRACT

ATTACHED

DISTRIBUTION STATEMENT A
Approved for Public Release
Distribution Unlimited

20040423 017

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
				8	Leszek Demkowicz
					19b. TELEPHONE NUMBER (Include area code): 512-471-4199

Abstract
Fully Automatic, hp-Adaptive Simulations for Maxwell's Equations
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The report describes a computational and theoretical work toward developing a fully automatic hp-adaptive methodology for solving 3D time-harmonic Maxwell equations. The algorithm produces automatically a sequence of hp meshes that deliver exponential convergence. The optimal hp-refinements are identified by minimizing the projection based interpolation error of the solution obtained on a (fine) grid obtained by a global hp-refinement of a current (coarse) grid.

The idea of the algorithm is very general and it applies to all discretizations forming the hp de Rham diagram - H1- H(curl)-and H(div)-conforming.

Final report for the project on

Fully Automatic, *hp*-Adaptive Simulations for Maxwell's Equations.

1 Accomplishments of the project. A summary

The project was a continuation of an earlier, three-year project on "An *hp* Adaptive Finite Element Simulator for Maxwell's Equations with Application to 3-D Scattering and Resonating Cavities Problems", during which a new Finite Element Method allowing for variable mesh size h and order of approximation p, was proposed and studied. The new element was shown to belong to a general family of conforming elements forming an exact sequence, and a family of projection-based interpolation operators was constructed that make the de Rham diagram commute. Two pilot codes, 2D (triangles,quads), and 3D (hexahedra) were built, and a number of model, test cases was solved. The possibility of achieving an exponential convergence for problems with singular solutions was demonstrated through numerical experiments.

In the presented project, the crucial task of working out a fully automatic *hp*-adaptive strategy that would deliver the exponential convergence for solving time-harmonic Maxwell equations, was undertaken. The work combined, in a very "tied loop", development of a new, fundamental mathematical theory, with a professional quality code development. The two sides of the project - theory and code building, strongly influence each other. Without any exaggeration, it would have been impossible to develop the projection-based interpolation theory without the experience gained during the computations, with the theory in turn, providing theoretical foundations for the mesh optimization algorithm .

1.1 Theory

The concept of elements of variable order forming the exact sequence, with the projection-based interpolation operators satisfying the commuting diagram property, was generalized to Nedelec simplices of the first kind [4]. Out of all Nedelec elements, only one (hexahedra and quads of the second type), do not satisfy the exact sequence property, and fail to converge. Generalizations of all remaining elements to the variable order of approximation setting, is discussed in [11, 12]. The optimal p and *hp* interpolation estimates were derived in [5] for triangular meshes. The 3D interpolation theory is much more advanced and different principles have to be used [13, 14]. While the interpolation theory for elliptic problems is complete, the theory for $H(curl)$- and $H(div)$-conforming discretizations hinges on a single conjecture on existence of 3D polynomial preserving

extension operators for $H(curl)$ spaces.

Extensions to non-simplicial elements are rather straightforward, and we plan to do it in a near future.

In a separate effort, we have been studying the discrete compactness property for the p and hp methods. This crucial property implies convergence of eigenvalues and, therefore, stability of FE discretizations of time-harmonic Maxwell equations as well. Some preliminary results for a triangular element, obtained under a L^2 -discrete stability conjecture, were reported in [2]. I am happy to inform that the results have been recently extended to the quad element (paper in completion).

1.2 Code development and problems solved

The original, proof of concept codes, developed with Rachowicz [3], have been rewritten within a completely new data structure [7, 8]. The codes survived the ultimate test of supporting the automatic *hp*-adaptivity and a two-grid solver. Since last Summer, the codes are maintained on the Web under CVS with current updates available immediately to computational math community. The number of national and international users is steadily growing. Most of the coding is done in collaboration with Waldek Rachowicz from Cracow and Adam Zdunek from Stockholm.

The two principal components of this project are the automatic *hp*-adaptivity module and the two grid solver. The 2D mesh optimization module has undergone four iterations [6, 9, 10] and it is operational for both elliptic and Maxwell problems. The methodology has been successfully tested on tvelwe non-trivial test examples including orthotropic heat conduction, elasticity, acoustic and electromagnetic scattering problems, and wave propagation in conductive media.

It took two and a half years to complete the 3D mesh optimization module which has been so far tested only on two elliptic examples. A second implementation of the 3D mesh optimization module is underway (a Ph.D. project of Jason Kurtz). We anticipate presenting solutions to the 3D scattering problems obtained with the automatic *hp*-refinements algorithm, during the next Air Force workshop (2005).

Crucial to the success of the proposed methodology is the two-grid solver that makes the solution of the fine grid problem possible. The work has been summarized in [17] and in dissertation of David Pardo [18], to be defended on April 2, 2004.

In summary, on the code development side, we are about a year late, compared with the initial plans.

In a parallel effort, the automatic *hp*-adaptivity algorithm has been coupled with the goal-oriented mesh optimization [20], and the 2D elliptic code has been successfully parallelized for memory distributed platforms.

2 Publications acknowledging the Air Force support

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[1] M. Ainsworth, and L. Demkowicz, "Explicit Polynomial Preserving Trace Liftings on a Triangle", *ICES Report 03-47.*

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[5] L. Demkowicz, and I. Babuška, "Optimal p Interpolation Error Estimates for Edge Finite Elements of Variable Order in 2D", *SIAM J. Numer. Anal.* **41**,4, 1195-1208, 2003.

[6] L. Demkowicz, W. Rachowicz, and Ph. Devloo, "A Fully Automatic hp-Adaptivity", *Journal of Scientific Computing*; **17**(1-3): 127-155.

[7] L. Demkowicz, "2D hp-Adaptive Finite Element Package (2Dhp90). Version 2.0", *TICAM Report 02-06*, Jan 02.

[8] L. Demkowicz, D. Pardo, W. Rachowicz, "3D hp-Adaptive Finite Element Package (3Dhp90). Version 2.0, The Ultimate Data Structure for Three Dimensional, Anisotropic hp Refinements", *TICAM Report 02-24.*

[9] L. Demkowicz, "*hp*-Adaptive Finite Elements for Time-Harmonic Maxwell Equations", in *Topics in Computational Wave Propagation*, M. Ainsworth, P. Davies, D. Duncan, P. Martin, B. Rynne (Eds.), Lecture Notes in Computational Science and Engineering, Springer Verlag, Berlin 2003.

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[11] L. Demkowicz "Finite Element Methods for Maxwell Equations" *Encyclopedia of Computational Mechanics* (eds. E. Stein, R. de Borst, T.J.R. Hughes), Wiley and Sons, 2003, accepted.

[12] L. Demkowicz, "Exact Sequences, de Rham Diagram, Maxwell Equations, and hp-Adaptivity", *Proceedings of 15th International Conference on Computer Methods in Mechanics*, CMM-2003, Wisla, Poland, Jun 3-6, 2003 (invited plenary talk)

[13] L. Demkowicz, "Projection Based Interpolation", *ICES Report 04/03.*

[14] L. Demkowicz and A. Buffa, "$H^1, \boldsymbol{H}$(curl) and $\boldsymbol{H}$(div)-Conforming Projection-Based Interpolation in Three Dimensions", *ICES Report*, in preparation.

[15] J. Gopalakrishnan and L. Demkowicz, "Quasioptimality of Some Spectral Mixed Methods" *SIAM Journal on Numerical Analysis*, accepted.

[16] J. Gopalakrishnan, L.E. Garcia-Castillo, and L. Demkowicz, "Nedelec Spaces in Affine Coordinates" *Computers and Mathematics with Applications*, accepted.

[17] D. Pardo, L. Demkowicz, "Integration of *hp* Adaptivity and Multigrid. I. A Two Grid Solver for *hp* Finite Elements", *TICAM Report 02-33*, Sep 02.

[18] D. Pardo, "Integration of *hp* Adaptivity With a Two Grid Solver. Applications to Electromagnetics", Ph. D. Dissertation, University of Texas at Austin, available at *www.ices.utexas.edu/~pardo*

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[20] P. Solin, L. Demkowicz, "Goal Oriented *hp* Adaptivity for Elliptic Problems", *Computer Methods in Applied Mechanics and Engineering*, accepted.

3 Presentations acknowledging the Air Force support

1. L. Demkowicz, "Adaptive hp FE Modeling For Maxwell's Equations", Worcester Polytechnic Institute Mathematical Science Colloquium, Nov 10, 2000 (invited seminar).

2. L. Demkowicz, "Adaptive hp FE Modeling For Maxwell's Equations", Penn State University, Dept. of Mathematics, Applied and Computational Mathematics Series, December 8, 2000 (invited seminar).

3. L. Demkowicz, "Adaptive hp FE Modeling For Maxwell's Equations, A progress Report", AFOSR Electromagnetic Workshop, San Antonio, Jan 11- Jan 13, 2001.

4. L. Demkowicz "Adaptive hp FE Modeling For Maxwell's Equations, A progress Report", GAMM Workshop on Computational Electromagnetics, Kiel, Jan 26 - Jan 28, 2001 (invited talk).

5. L. Demkowicz "Adaptive hp FE Modeling For Maxwell's Equations", Applied and Computational Mathematics Seminar, University of California at Irvine, Feb 23, 2001.

6. L. Demkowicz, "Optimal p Interpolation Error Estimates for Edge Finite Elements of Variable Order in 2D", FE Rodeo, Southern Methodist University, Dallas, Mar.2-Mar.3,

7. L. Demkowicz, "Optimal p Interpolation Error Estimates for Edge Finite Elements of Variable Order in 2D", Brown University, Division of Applied Mathematics, Scientific Computing Seminar, Mar. 23, 2001, (invited talk).

8. L. Demkowicz, "Adaptive hp Modeling for Time Harmonic Maxwell's Equations. A Progress Report", International Conference on Spectral and Higher Order Methods, (ICOSAHOM-01), Upsalla, Jun. 10-Jun. 16, 2001 (invited plenary talk).

9. Bajer, A., Rachowicz, W., Walsh, T., L. Demkowicz, "A Two-Grid Parallel Solver for Time Harmonic Maxwell's equations and hp Meshes", Second European Conference on Computational Mechanics, Cracow, Jun.25 - Jun.29, 2001.

10. L. Demkowicz, "hp Interpolation Error Estimates for Maxwell's Equations in 2D", Second European Conference on Computational Mechanics, Cracow, Jun.25 - Jun.29, 2001.

11. L. Demkowicz, Rachowicz, W., Cecot, W., "A Three-Dimensional Infinite Element Method for Maxwell's Equations", Sixth U.S. National Congress on Computational Mechanics, Dearborn, Michigan, July 31-Aug 4, 2001.

12. L. Demkowicz, "Electromagnetic Device Modeling Using hp-Adaptive Edge Finite Elements", Schlumberger, Sugar Land, August 8, 2001.

13. L. Demkowicz, "hp-Adaptive Finite Element Methods. Part 1: de Rham Diagram, Part 2: Optimal hp Interpolation, Part 3: Automatic hp-Adaptivity, *hp* Data Structures" TICAM Seminar, Sep. 6,11,13,18, 01.

14. L. Demkowicz, "Fully Automatic hp-Adaptive Finite Element Simulations for Maxwell's Equations", AFOSR Electromagnetics Workshop, San Antonio, Jan 17-19, 02.

15. L. Demkowicz, "Fully Automatic hp-Adaptive Finite Elements. Integration of hp- Adaptivity with a Multigrid Solver", Seminari di Analisi Numerica, Dipartimento di Matematica, Pavia, Feb. 26, 2002

16. L. Demkowicz, "hp-Adaptive Finite Element Methods with Applications to Electromagnetics and Acoustics", NPACI AHM2002, San Diego, Mar 6-8, 2000 (invited plenary talk)

17. L. Demkowicz, "Fully Automatic hp-Adaptive Simulations for Maxwell's Equations" Air Force Institute of Technology, Department of Mathematics and Statistics Seminar, Apr 11, 2002 (invited seminar).

18. Leszek Demkowicz, David Pardo, "Integration of hp-Adaptivity with a Multigrid Solver", 14th US National Congress of Theoretical and Applied Mechanics, Blacksburg, VA, Jun 23-28, 2002.

19. Leszek Demkowicz, "Fully Automatic hp-Adaptive Simulations for Maxwell's Equations", Workshop on Computational Electromagnetics, Baltimore, Jun 27-28, 2002 (invited talk).

20. Leszek Demkowicz, "hp-Adaptive Finite Element Methods", three seminars delivered at Jagiellonian University, Cracow University of Technology and Academy of Mining and Steel Works, in Cracow, Jul 1-5, 2002.

21. Leszek Demkowicz, David Pardo and Waldek Rachowicz, "Fully Automatic hp-Adaptive Finite Elements. Integration of hp-Adaptivity with a Multigrid Solver", Fifth World Congress on Computational Mechanics (WCCM V) Vienna, Jul 7-12, 2002.

22. Leszek Demkowicz, "Fully Automatic hp-Adaptive Finite Elements for Time-Harmonic Maxwell's Equations", LMS Durham Symposium on Computational Methods for Wave Propagation in Direct Scattering Durham, England, July 15-25 2002 (a series of three invited lectures).

23. Leszek Demkowicz, "Fully Automatic hp-Adaptive Simulations" IMACS workshop on "Adaptive Methods for PDE", the Fields Institute for Research in Mathematical Sciences, Toronto, Canada, 6-9 August 2002 (invited talk).

24. Leszek Demkowicz, "Fully Automatic hp-Adaptive Finite Element Simulations for Maxwell's Equations", Shlumberger, Sugar Land, August 27, 2002.

25. L. Demkowicz, "Fully Automatic hp-Adaptive Simulations" Sandia Labs, Nov 12, 2002 (invited seminar).

26. L. Demkowicz, "Parallel hp-Adaptive FE Simulations of Electromagnetic Waves", Supercomputing 2002, Baltimore, Nov 19, 2002.

27. L. Demkowicz, D. Pardo, "Fully Automatic hp-Adaptive Simulations for Maxwell's Equations", AFOSR Electromagnetics Workshop, San Antonio, Jan 9-11, 2003.

28. L. Demkowicz "Fully Automatic hp-Adaptive Simulations of Wave Propagation Problems", NPACI AHM, San Diego, Mar 19 (invited talk).

29. L. Demkowicz, "Exact sequences, de Rham diagram, Maxwell equations, and hp-adaptivity", 15th International Conference on Computer Methods in Mechanics, CMM-2003, Wisla, Poland, Jun 3, 2003 (invited plenary talk).

30. L. Demkowicz, "Fully Automatic hp-Adaptive Elements", Universitat der Bundeswehr Munchen Jun 11 (invited seminar).

31. L. Demkowicz, "Fully Automatic hp-Adaptive Elements", Technische Universitaet Muenchen, Jun 11 (invited seminar).

32. L. Demkowicz "Fully Automatic hp-Adaptive Simulations for Maxwell's Equations" International Workshop on "Numerical and Symbolic Scientific Computing, St. Wolfgang / Strobl (Austria), Jun 18, 2003 (an invited talk).

33. L. Demkowicz "hp-Adaptive Finite Elements, a Quest for Exponential Convergence" Eleventh conference on the Mathematics of Finite Elements and Applications (MAFELAP), Jun 22, 2003 (invited plenary talk)

34. L. Demkowicz "Fully Automatic hp-Adaptive Simulations for Maxwell's Equations" Eleventh conference on the Mathematics of Finite Elements and Applications (MAFELAP), Jun 22, 2003 (a presentation in minisymposium)

35. L. Demkowicz "Fully Automatic hp-Adaptive Simulations" Baker-Hughes, Houston, Jul 23 (invited seminar).

36. L. Demkowicz "hp-Adaptive Finite Element Codes at ICES" ICES Seminar, Jul 25, 2003.

37. L. Demkowicz "Exact Sequences, De Rham Diagram, Maxwell Equations, hp Adaptivity", 7th US National Congress on Computational Mechanics, Jul 29, 2003 (invited plenary talk).
38. L. Demkowicz "Fully Automatic hp-Adaptivity for Maxwell Equations" 7th US National Congress on Computational Mechanics, Jul 29, 2003 (minisymposium talk).
39. L. Demkowicz, "Fully Automatic hp-Adaptive Simulations for Maxwell's Equations in Three Dimensions", AFOSR Electromagnetics Workshop, 8-10 Jan 2004
40. L. Demkowicz, "Fully Automatic hp-Adaptive Simulations for Maxwell's Equations in Three Dimensions", Electromagnetics Workshop, Oberwolfach, Feb 22-28, 2004
41. L. Demkowicz, "Polynomial Extensions and Projection-Based Interpolation in Three Dimensions", Finite Element Rodeo, Austin, Texas, Mar 5-6, 2004

4 Dissertations related to the project

1. David Pardo, "Integration of *hp* Adaptivity With a Two Grid Solver. Applications to Electromagnetics" Ph.D. dissertation, University of Texas at Austin, to be defended on April 2, 2004 [18]

   Besides the Air Force workshop, David has presented his work at two international and two national conferences, and has given a number of invited seminars in U.S. and Spain. He will stay with me for a one year postdoctoral study sponsored by Baker-Hughes, to work on modeling of EM logging tools.

2. Jason Kurtz, "A Fully Automatic 3D *hp*-Adaptive Strategy for Elliptic and Maxwell Problems", a Ph.D. dissertation project, started in September 2003.